Supporting Information

Direct Synthesis of Triazines from Alcohols and Amidines using Supported Pt Nanoparticle Catalysts under acceptorless dehydrogenative methodology.

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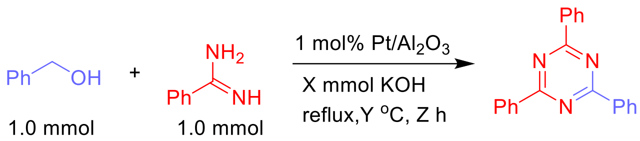
Table S1. Optimization of the reaction conditions for triazine synthesis from benzyl alcohol and benzamidine.



Entry No	Reduction temp (°C)	Solvent (2 mL)	Base (mmol)	Temp (°C)	Time (h)	Yield (%)
1	500	Toluene	KOH (0.1)	110	24	95
2	500	1,4-dioxane	KOH (0.1)	110	24	58
3	500	*o*-xylene	KOH (0.1)	110	24	78
4	500	DMSO	KOH (0.1)	110	24	75
5	500	Toluene	NaOH (0.1)	110	24	69
6	500	Toluene	KO^tBu (0.1)	110	24	88
7	500	Toluene	Cs_2CO_3 (0.1)	110	24	45
8	500	Toluene	KOH (0.1)	70	24	56
9	500	Toluene	KOH (0.1)	80	24	68
10	500	Toluene	KOH (0.1)	90	24	78
11	500	Toluene	KOH (0.1)	100	24	89
12	500	Toluene	KOH (0.1)	120	24	91
13	500	Toluene	KOH (0.1)	130	24	82
14	100	Toluene	KOH (0.1)	110	24	57
15	300	Toluene	KOH (0.1)	110	24	81
16	700	Toluene	KOH (0.1)	110	24	86

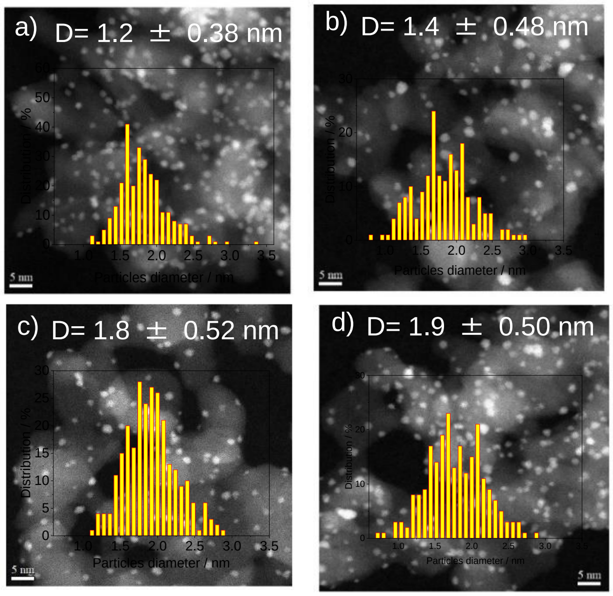


Figure S1: TEM images and histograms for Pt/Al_2O_3 catalysts reduced at a) 100 °C b) 300 °C c) 500 °C d) 700 °C

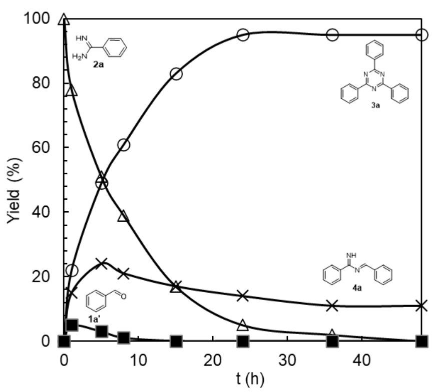
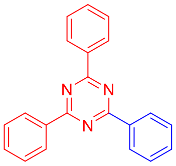


Figure S2: Time course profile for the synthesis of triazine

NMR and GC/MS analysis

^1H and ^{13}C NMR spectra were assigned and reproduced to the corresponding literature. ^1H and ^{13}C NMR spectra were recorded using at ambient temperature on JEOL-ECX 400 operating at 400.17 and 100.92 MHz, respectively with tetramethyl silane as an internal standard. Abbreviations used in the NMR experiments: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet, br, broad singlet. GC-MS spectra was taken by SHIMADZU QP2010.

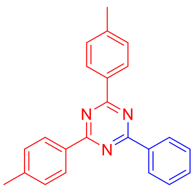
1,3,5-triphenyltraizine:[1]



3a

^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 8.79 (dd, *J*= 7.96 Hz, 6H), 7.55-7.62 (m, 9H), 8.02 (s, 1H), ^{13}C NMR (150.92 MHz, $CDCl_3$): δ 171.67, 136.26, 132.50, 128.97, 128.64.; GC-MS m/e 309.15.

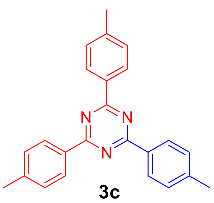
2,4-diphenyl-6-(*p*-tolyl)-1,3,5-triazine:[1]



3b

^{1}H NMR (400 MHz, CDCl3) δ 7.7-7.75 (d, J = 9.6 Hz, 6H), 7.57-7.46 (m, 7H), 1.68 (s, 6H) ^{13}C NMR (100 MHz, CDCl3) δ 176.88, 164.71, 132.41, 131.63, 128.49, 127.06, 25.01; GC-MS m/e 323.10.

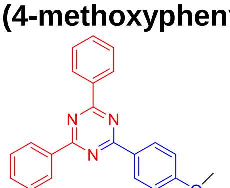
2,4,6-tri-*p*-tolyl-1,3,5-triazine:[1,2]



3c

^{1}H NMR (400 MHz, CDCl3) δ 7.73-7.69 (d, J = 8.9 Hz, 6H), 7.37-7.35 (d, J = 7.6 Hz, 6H), 2.40 (s, 9H) ^{13}C NMR (100 MHz, CDCl3) δ 169.50, 142.45, 130.48, 129.23, 127.34, 21.44; GC-MS m/e 351.20.

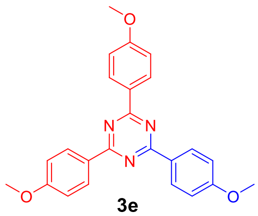
2-(4-methoxyphenyl)-4,6-diphenyl-1,3,5-triazine:[3,4]



3d

GC-MS m/e 339.10.

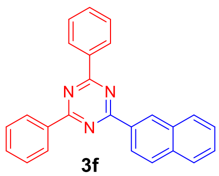
2,4,6-tris(*p*-methoxyphenyl)-1,3,5-triazine:[1]



3e

^{1}H NMR (400 MHz, DMSO-d6) δ 7.84- 8.82 (d, J = 9.6 Hz, 6H), 6.96-6.94 (d, J =8.4 Hz, 6H), 3.78 (s, 9H). ^{13}C NMR (100 MHz, CDCl3) δ 167.39, 161.53, 129.31, 126.48, 113.35, 55.28; GC-MS m/e 399.20.

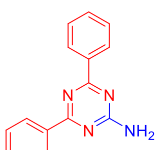
2-(naphthalen-2-yl)-4,6-diphenyl-1,3,5-triazine:[3]



3f

^{1}H NMR (400 MHz, CDCl3, TMS): δ 9.29 (s, 1H), 8.80 (d, J = 6.0 Hz, 5H), 8.09-7.90 (m, 3H), 7.64-7.53 (m, 8H), ^{13}C NMR (150.92 MHz, CDCl3): δ 171.62, 136.28, 135.67, 133.60, 133.09, 132.48, 129.99, 129.54, 128.99, 128.62, 128.28, 127.82, 126.42, 125.11; GC-MS m/e 359.4.

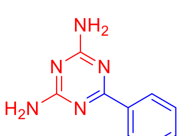
4,6-diphenyl-1,3,5-triazin-2-amine:



3g

^{1}H NMR (400 MHz, CDCl3) δ 7.83- 8.81 (d, J = 9.6 Hz, 4H), 7.56-7.43 (m, 6H), 6.16 (s, 2H). ^{13}C NMR (100 MHz, CDCl3) δ 169.47, 169.23, 133.33, 131.97, 128.60, 127.30; GC-MS m/e 248.10.

6-phenyl-1,3,5-triazine-2,4-diamine:[5]

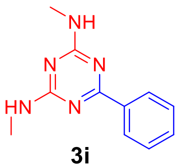


3h

^{1}H NMR (400 MHz, DMSO-d6, TMS): δ 8.22 (d, J = 8.8 Hz, 2H), 7.51-7.42 (m, 3H), 6.73

(s, 4H), ^{13}C NMR (100 MHz, CDCl3): δ 170.12, 167.43, 137.07, 130.97, 128.11, 127.64; GC-MS m/e 187.10.

N^2,N^4-dimethyl-6-phenyl-1,3,5-triazine-2,4-diamine:[6]



3i

GC-MS m/e 215.10.

Notes and references

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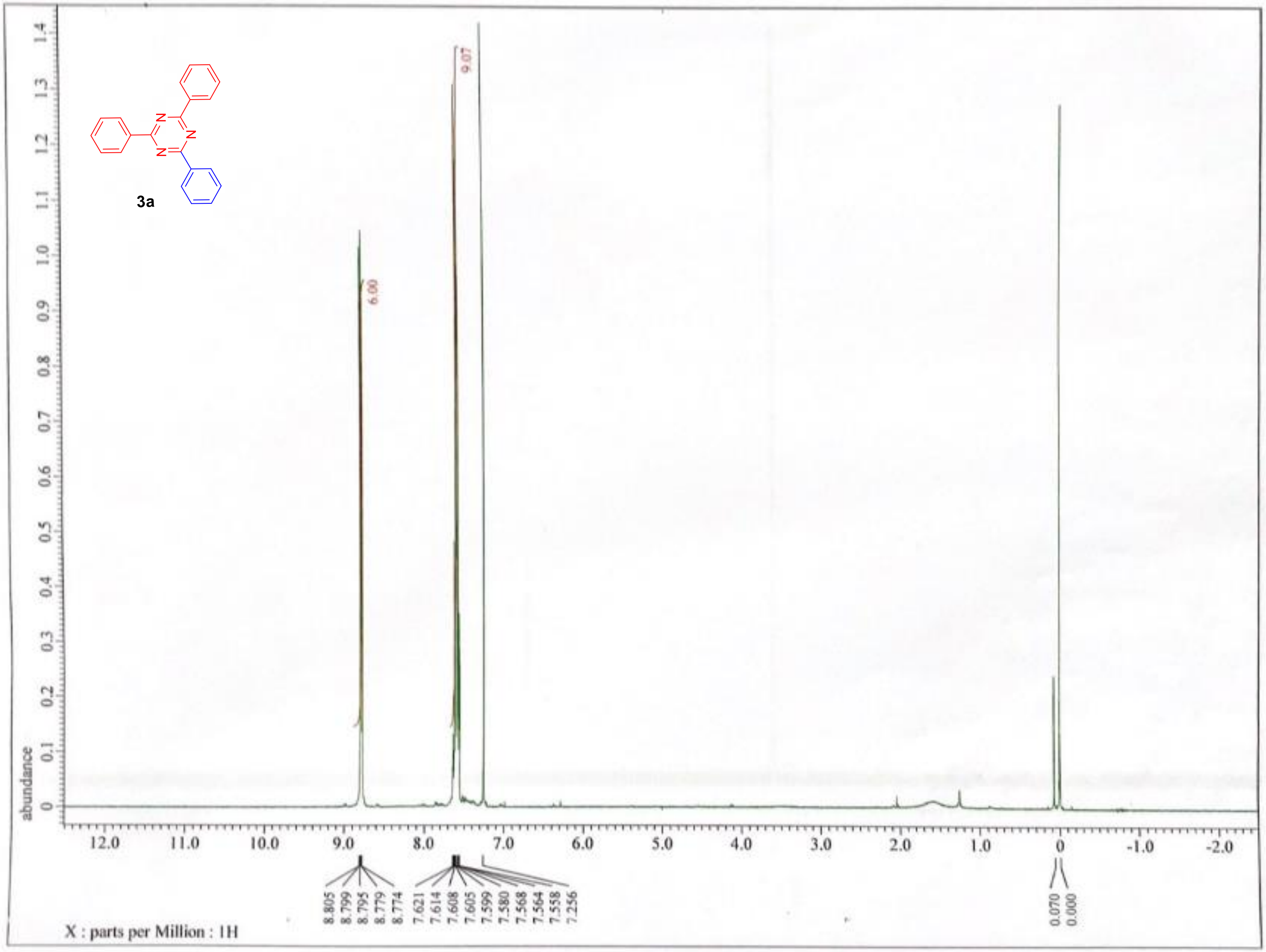

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
N
3a
6.00
9.07
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.805
8.799
8.795
8.779
8.774
7.621
7.614
7.608
7.605
7.599
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7.568
7.564
7.558
7.256
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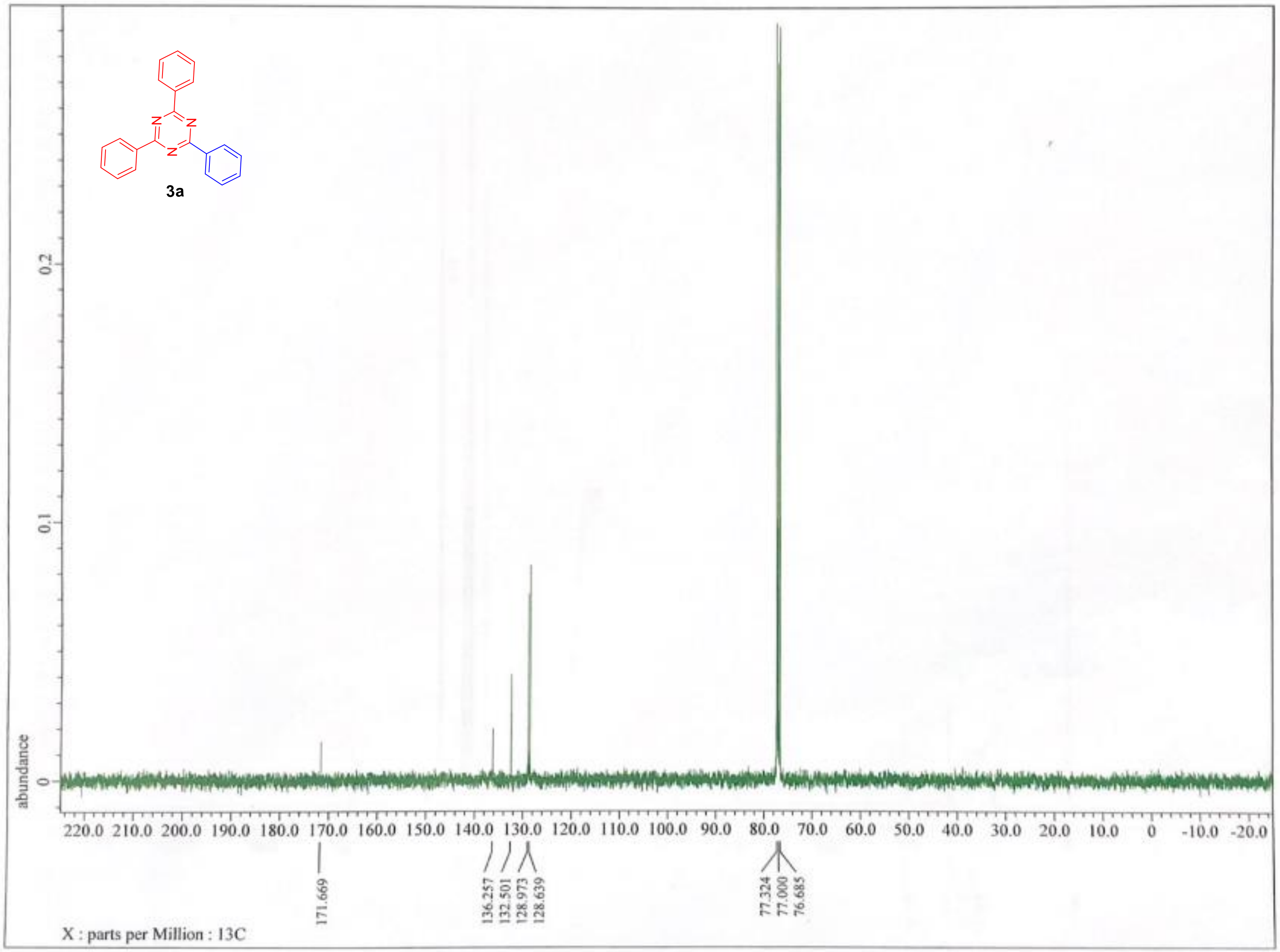
0.000
X : parts per Million : 1H



3a
abundance
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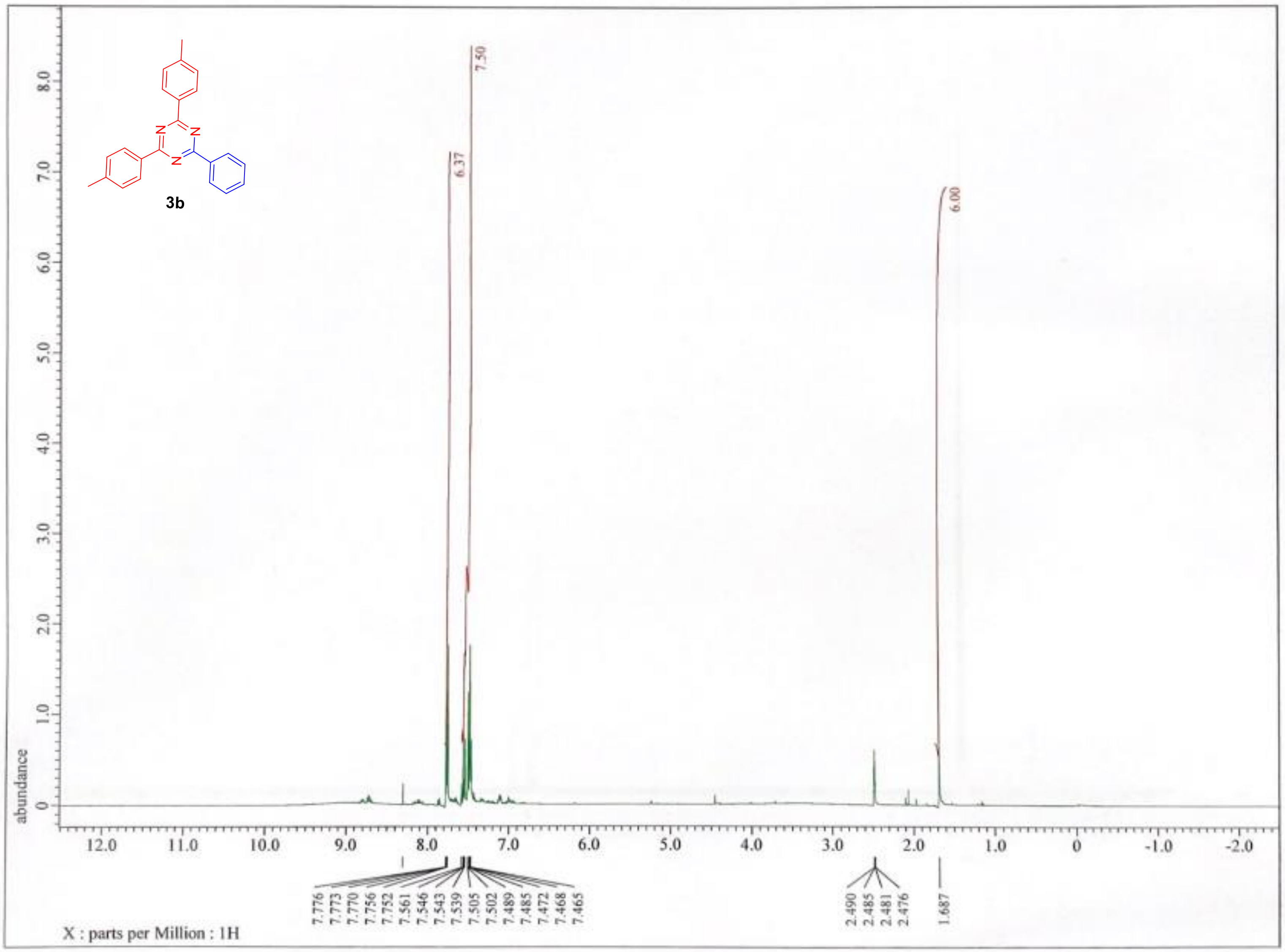
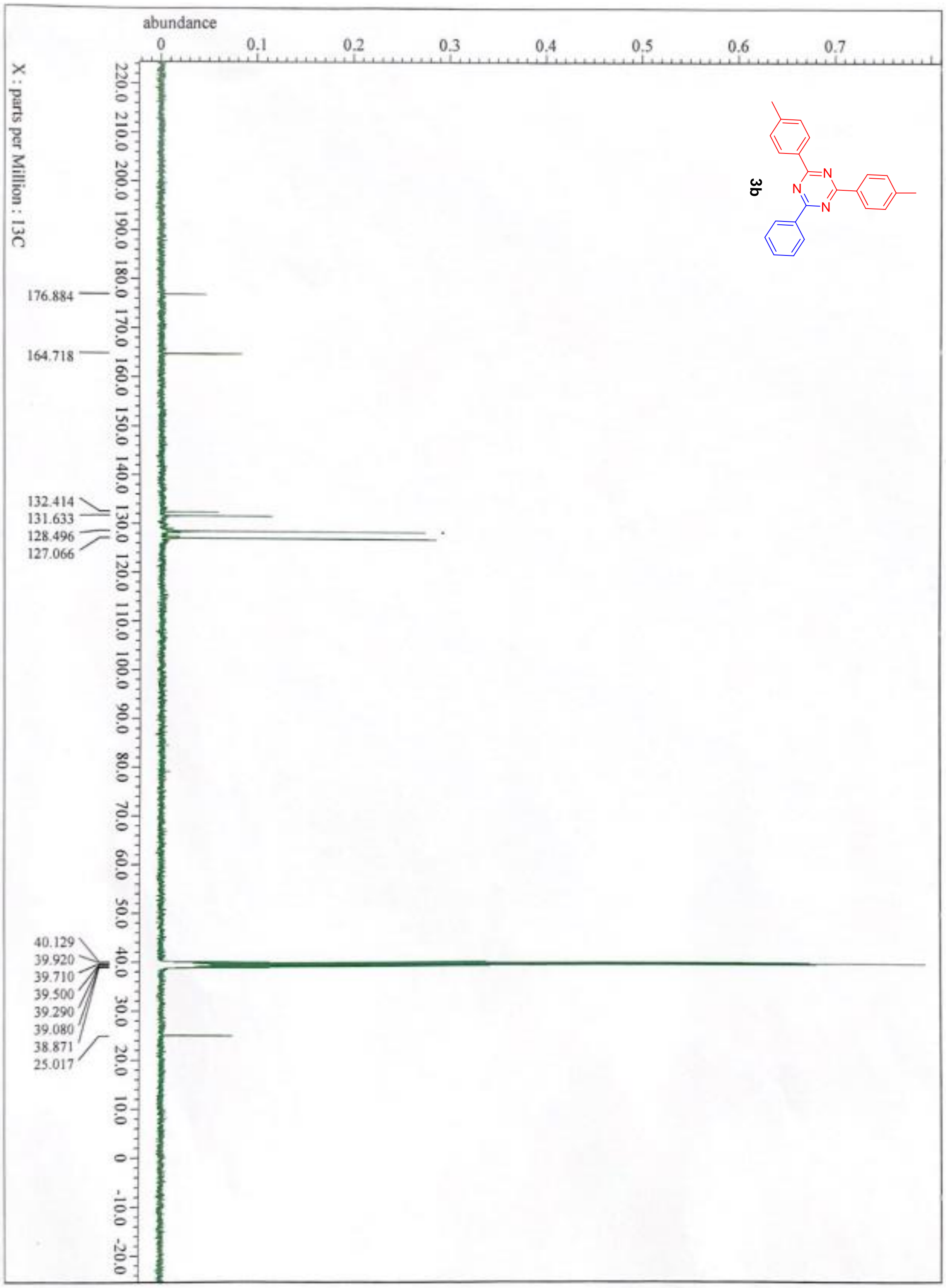
0.1
0.2
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
171.669
136.257
132.501
128.973
128.639
77.324
77.000
76.685
X : parts per Million : 13C



3b
abundance
X : parts per Million : 1H
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
7.776 7.773 7.770 7.756 7.752 7.561 7.546 7.543 7.539 7.505 7.502 7.489 7.485 7.472 7.468 7.465
2.490 2.485 2.481 2.476
1.687
6.37
7.50
6.00



abundance
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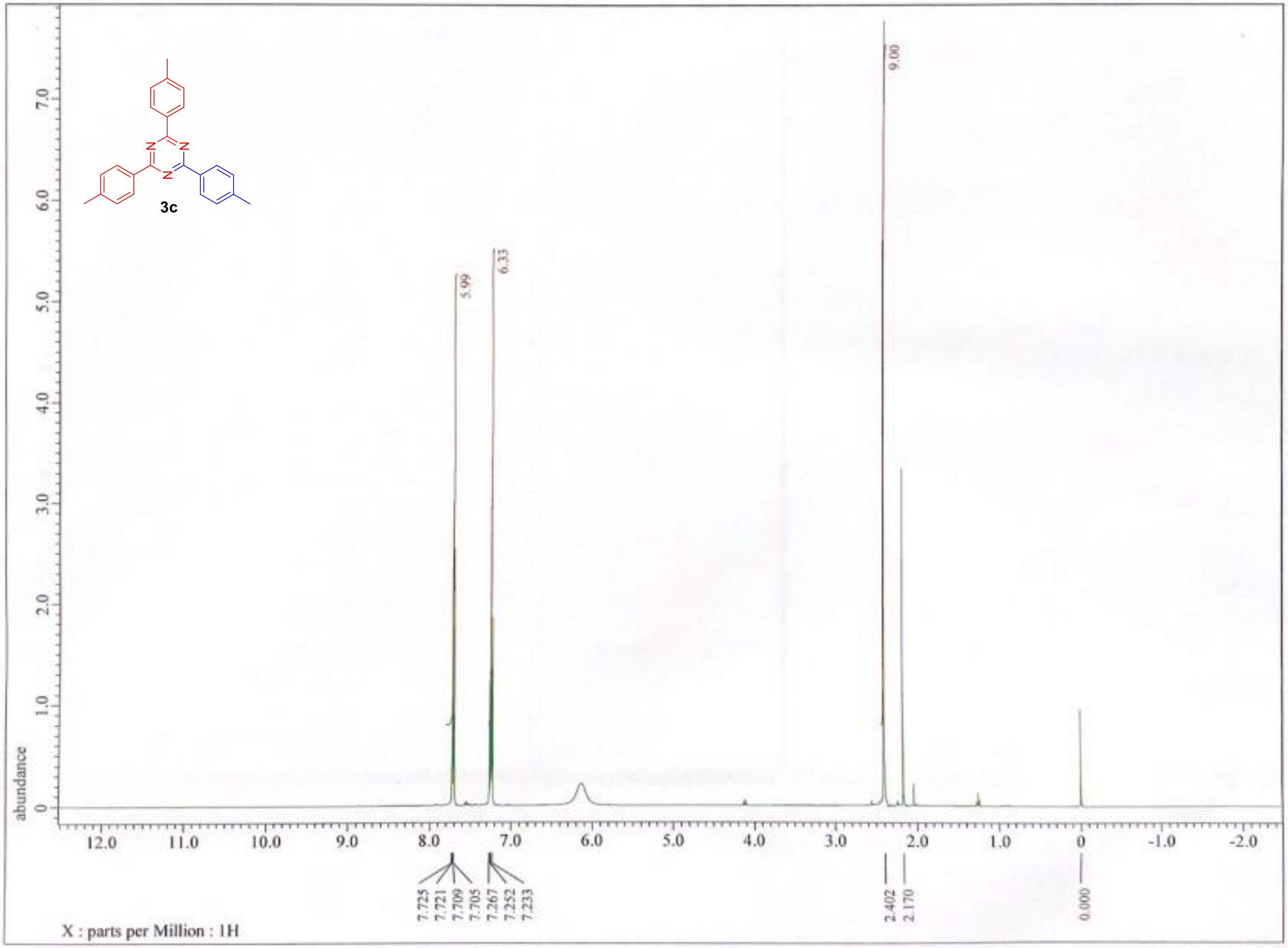
176.884
164.718
132.414
131.633
128.496
127.066
40.129
39.920
39.710
39.500
39.290
39.080
38.871
25.017
3b


3c
abundance
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0
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9.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
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7.709
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7.267
7.252
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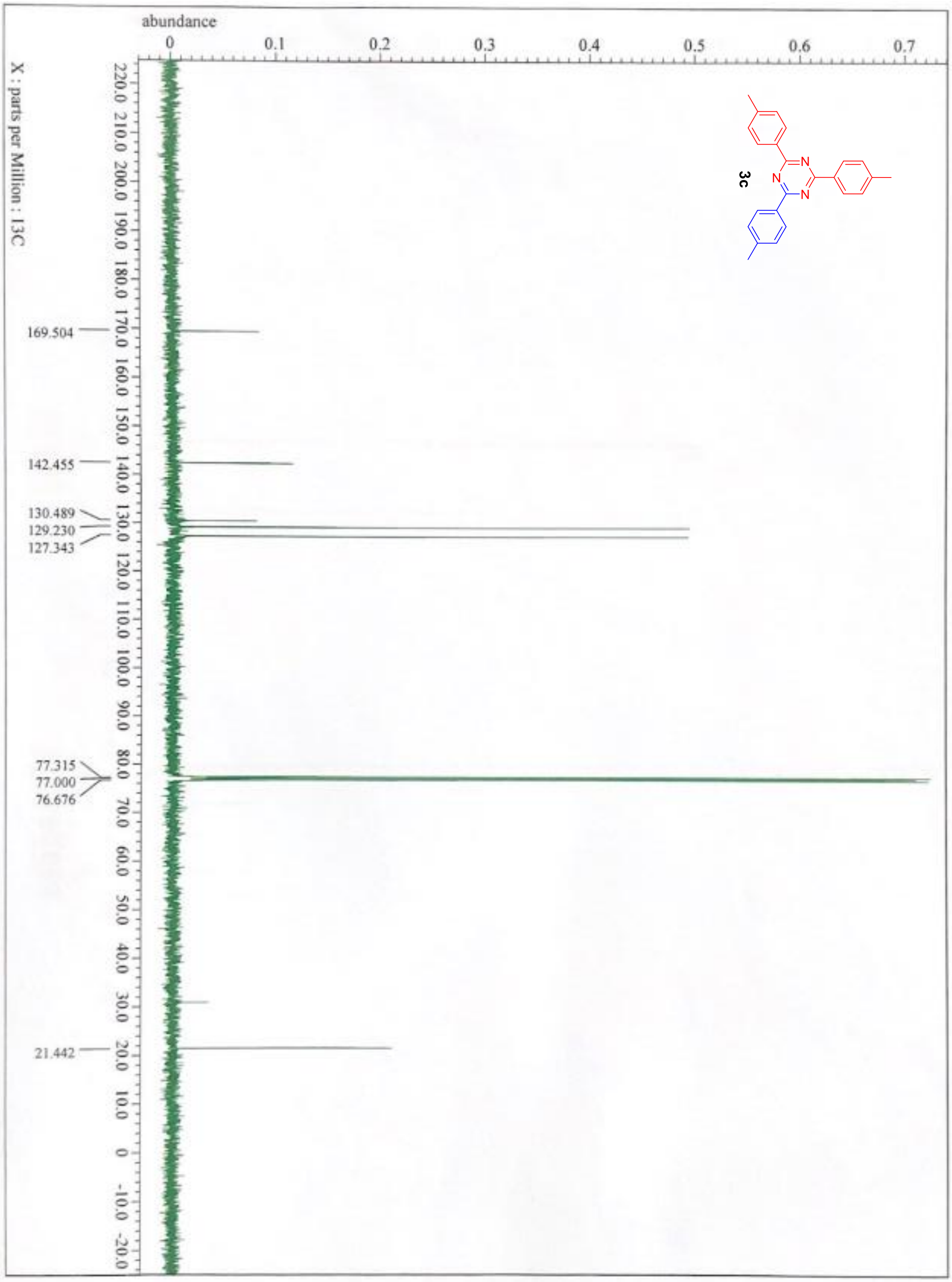
0.000
X : parts per Million : 1H



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0.3
0.4
0.5
0.6
0.7
X : parts per Million : 13C
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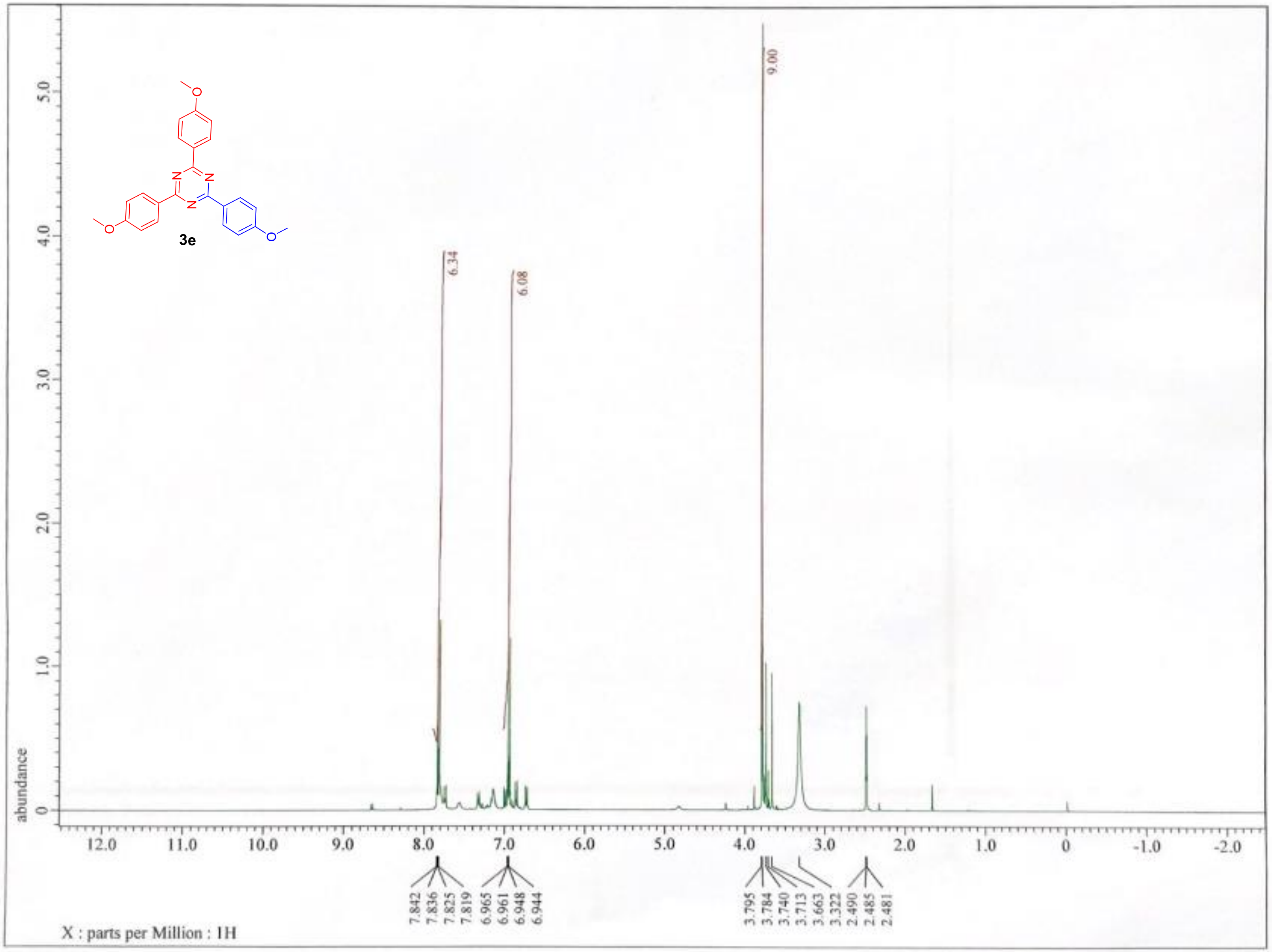
129.230
127.343
77.315
77.000
76.676
21.442
3c
N
N
N



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6.948
6.944
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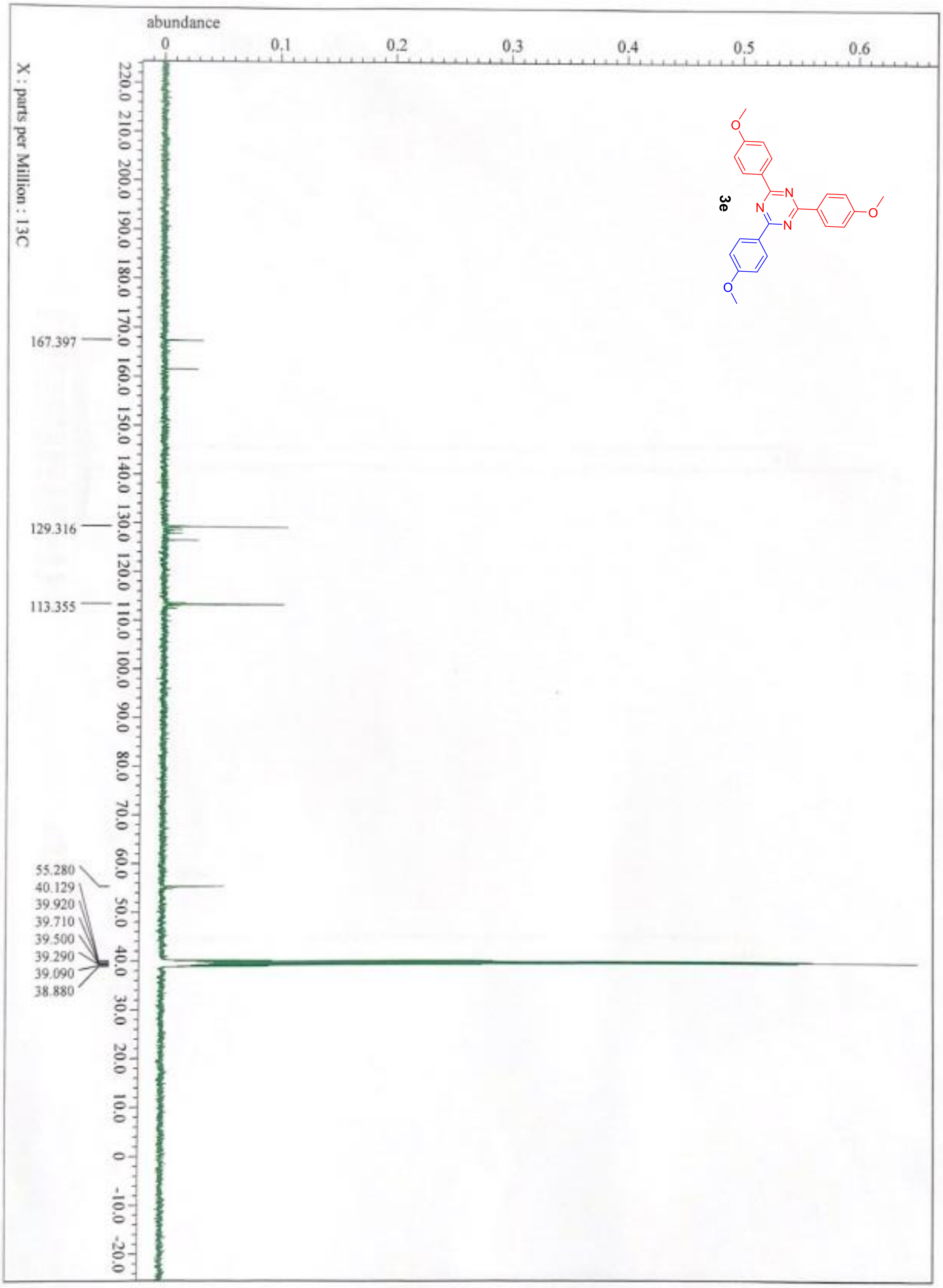
3.784
3.740
3.713
3.663
3.322
2.490
2.485
2.481
X : parts per Million : 1H



abundance
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0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
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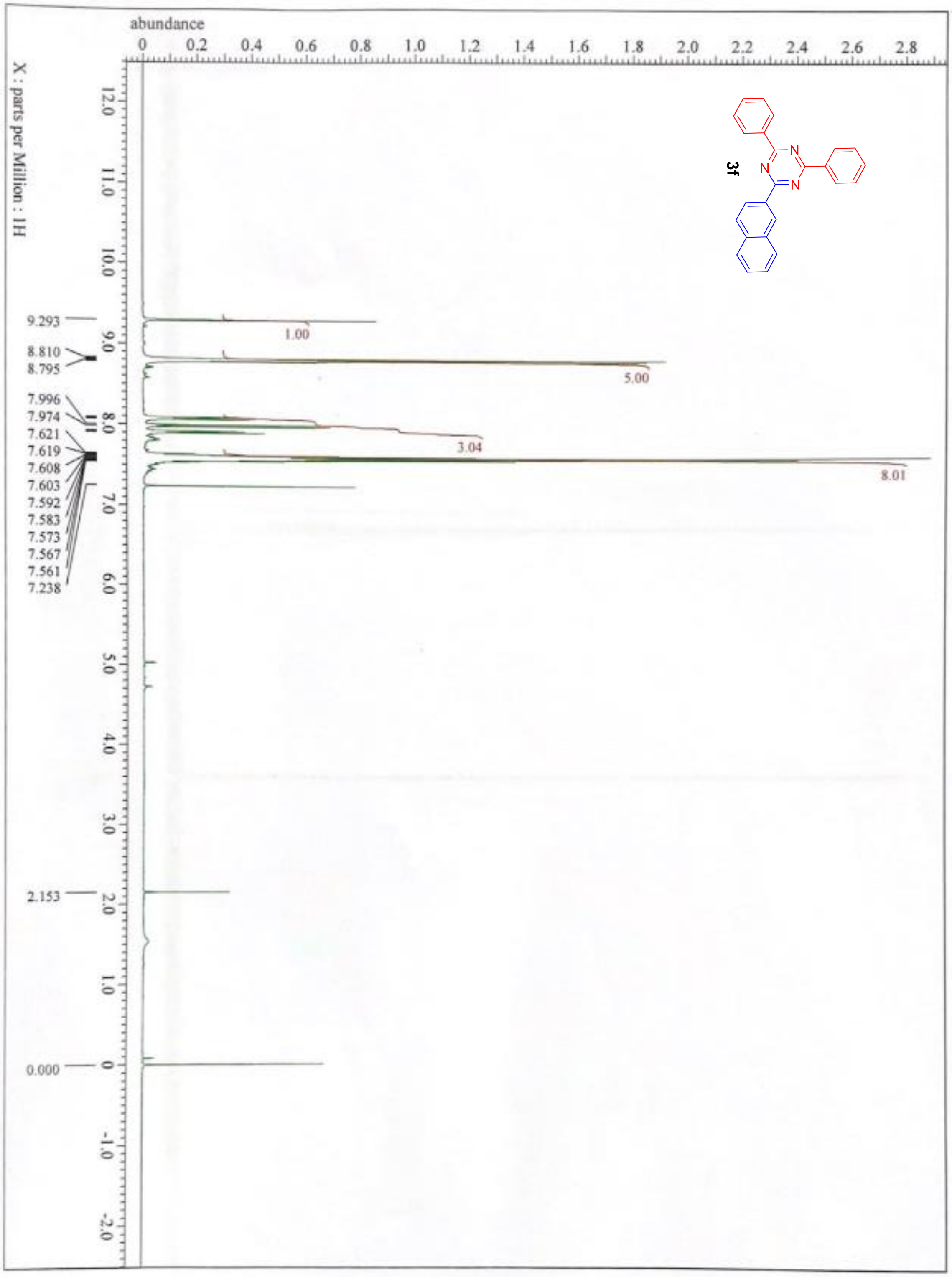
167.397
129.316
113.355
55.280
40.129
39.920
39.710
39.500
39.290
39.090
38.880
3e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X : parts per Million : 1H
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7.996
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7.621
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7.608
7.603
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7.561
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0.000
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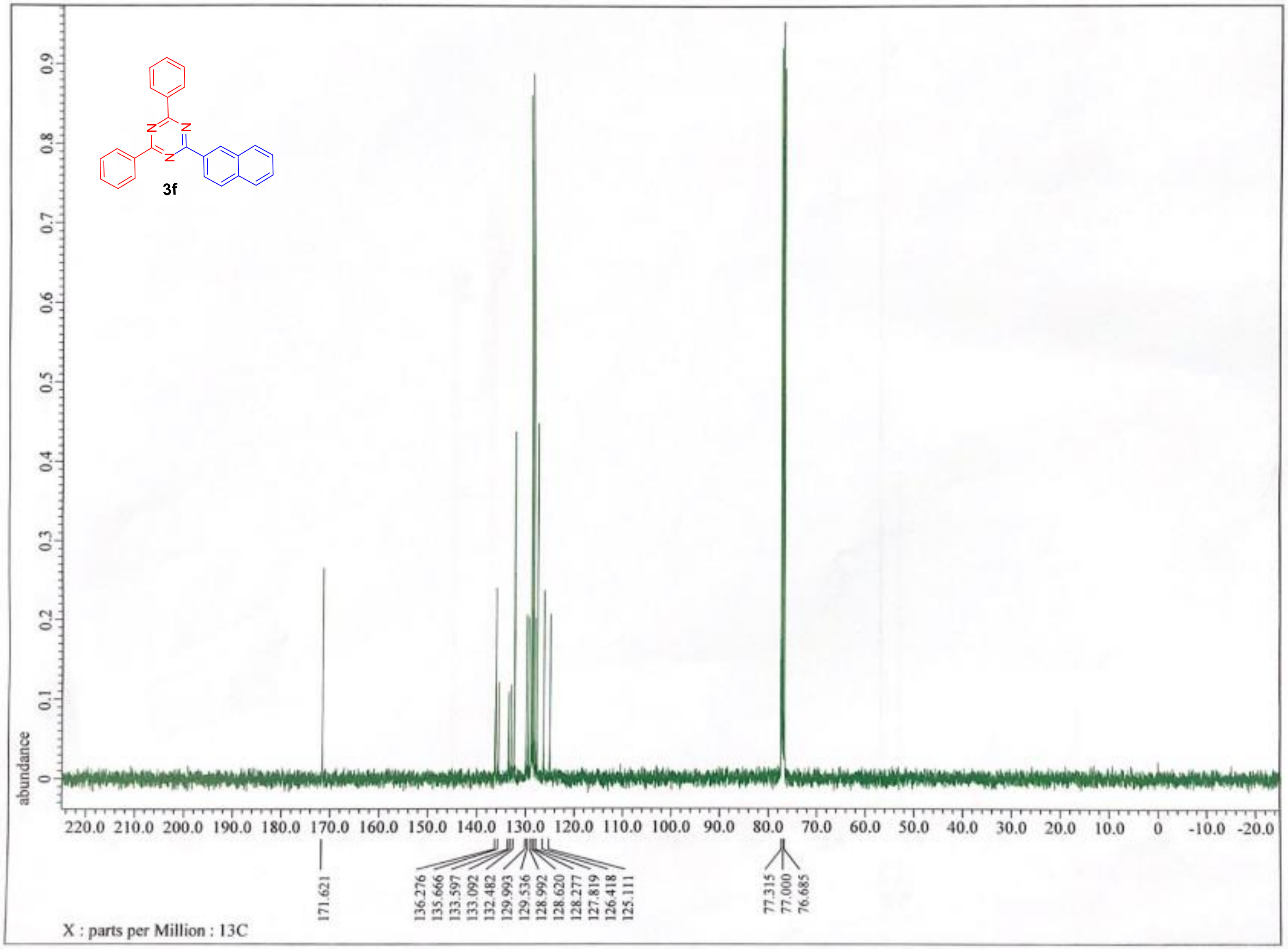
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0
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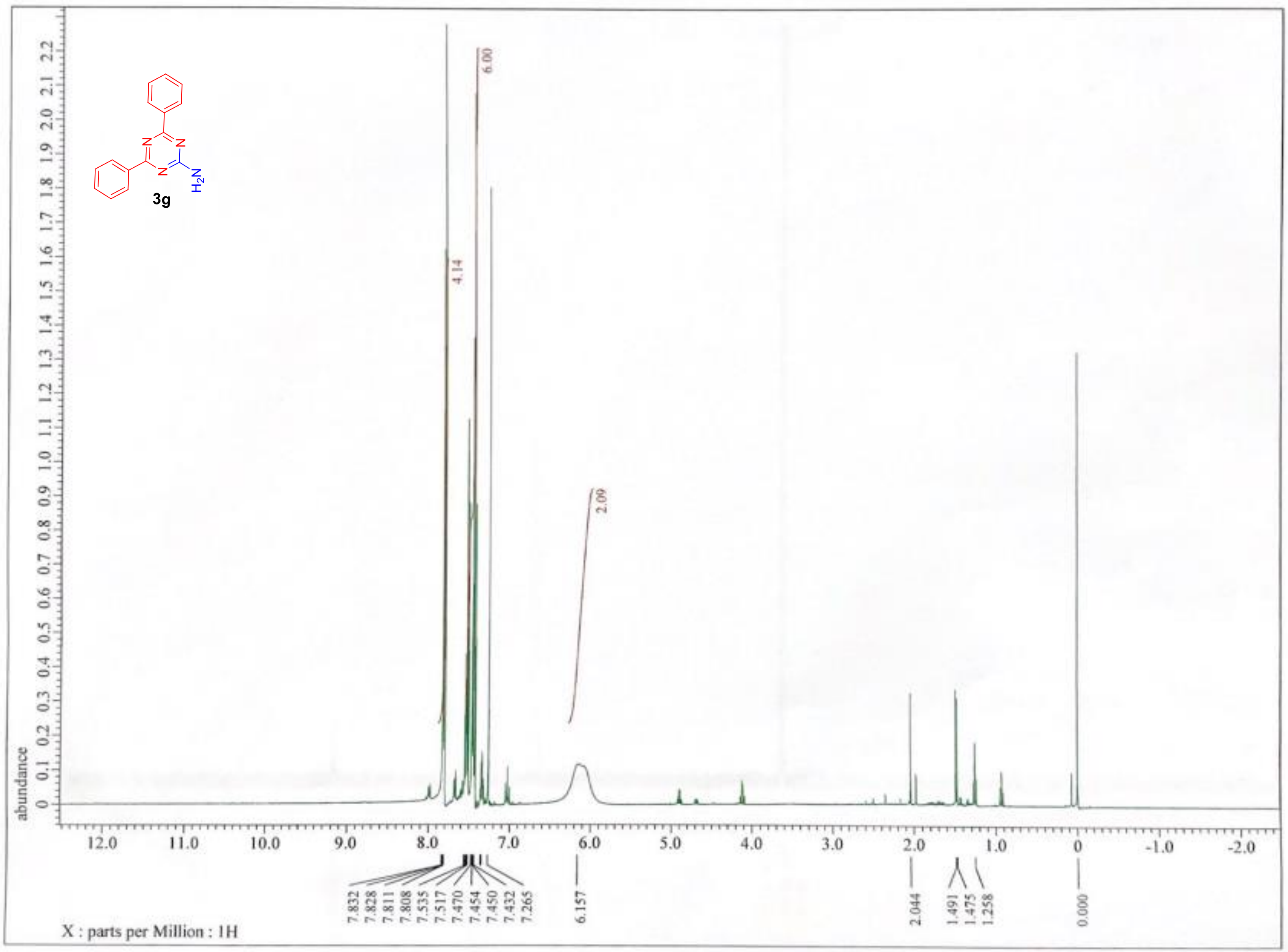
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
3f
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
171.621
136.276
135.666
133.597
133.092
132.482
129.993
129.536
128.992
128.620
128.277
127.819
126.418
125.111
77.315
77.000
76.685
X : parts per Million : 13C



3g
H2N
N
abundance
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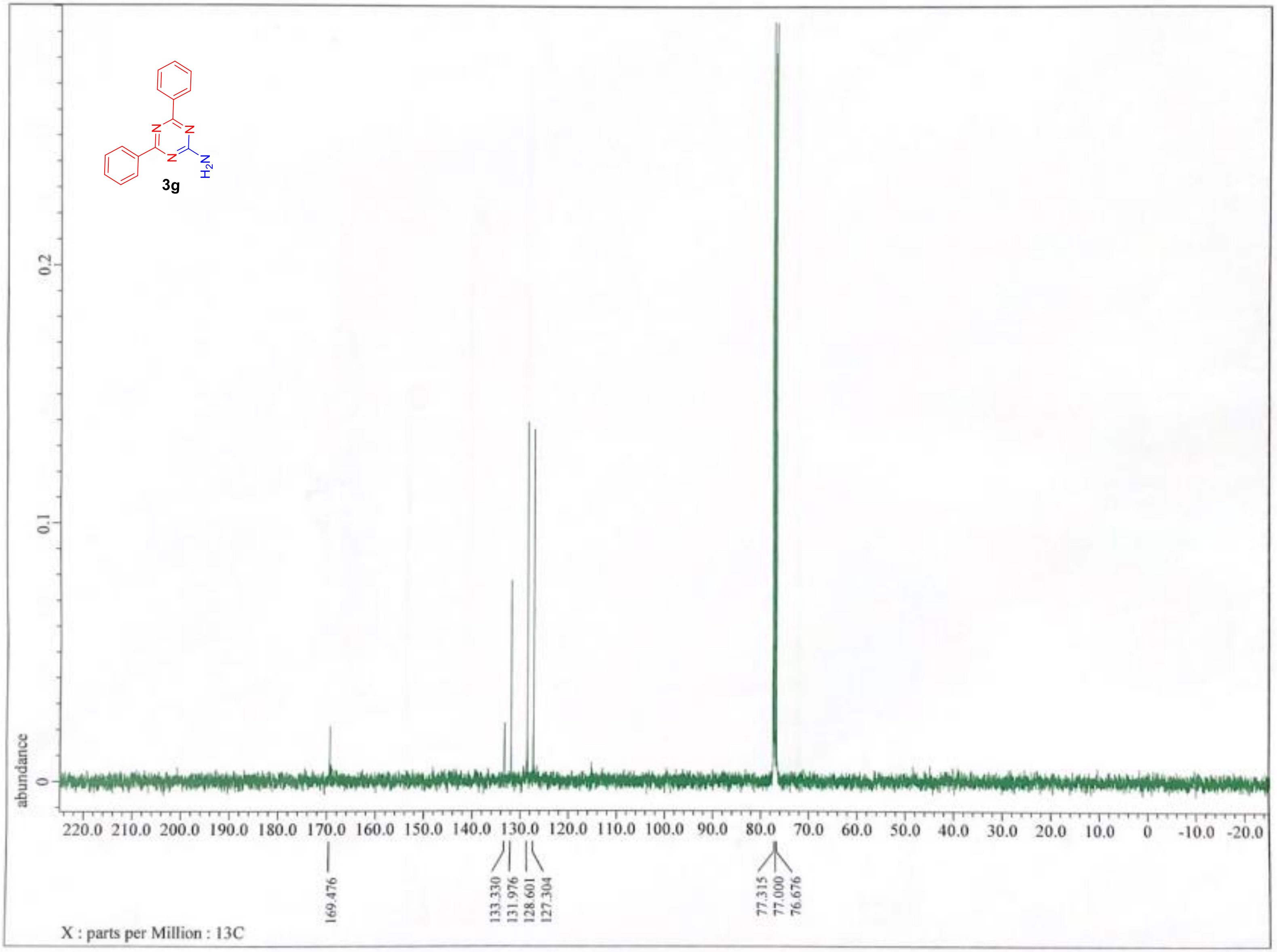
4.14
6.00
2.09
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
7.832 7.828 7.811 7.808 7.535 7.517 7.470 7.454 7.450 7.432 7.265
6.157
2.044
1.491 1.475 1.258
0.000
X : parts per Million : 1H



3g
H_2N
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0.2
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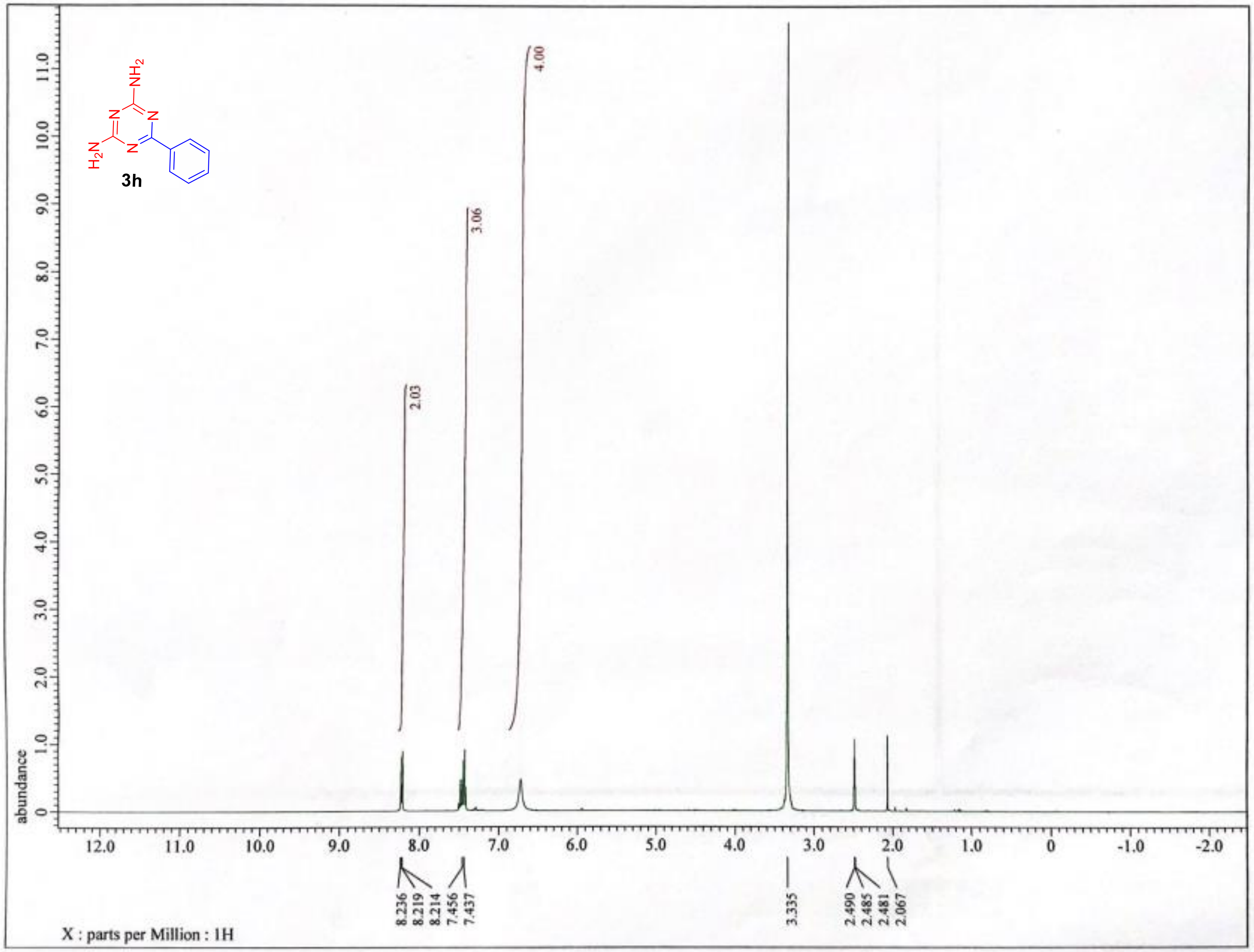
128.601
127.304
77.315
77.000
76.676
X : parts per Million : 13C



3h
abundance
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10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
2.03
3.06
4.00
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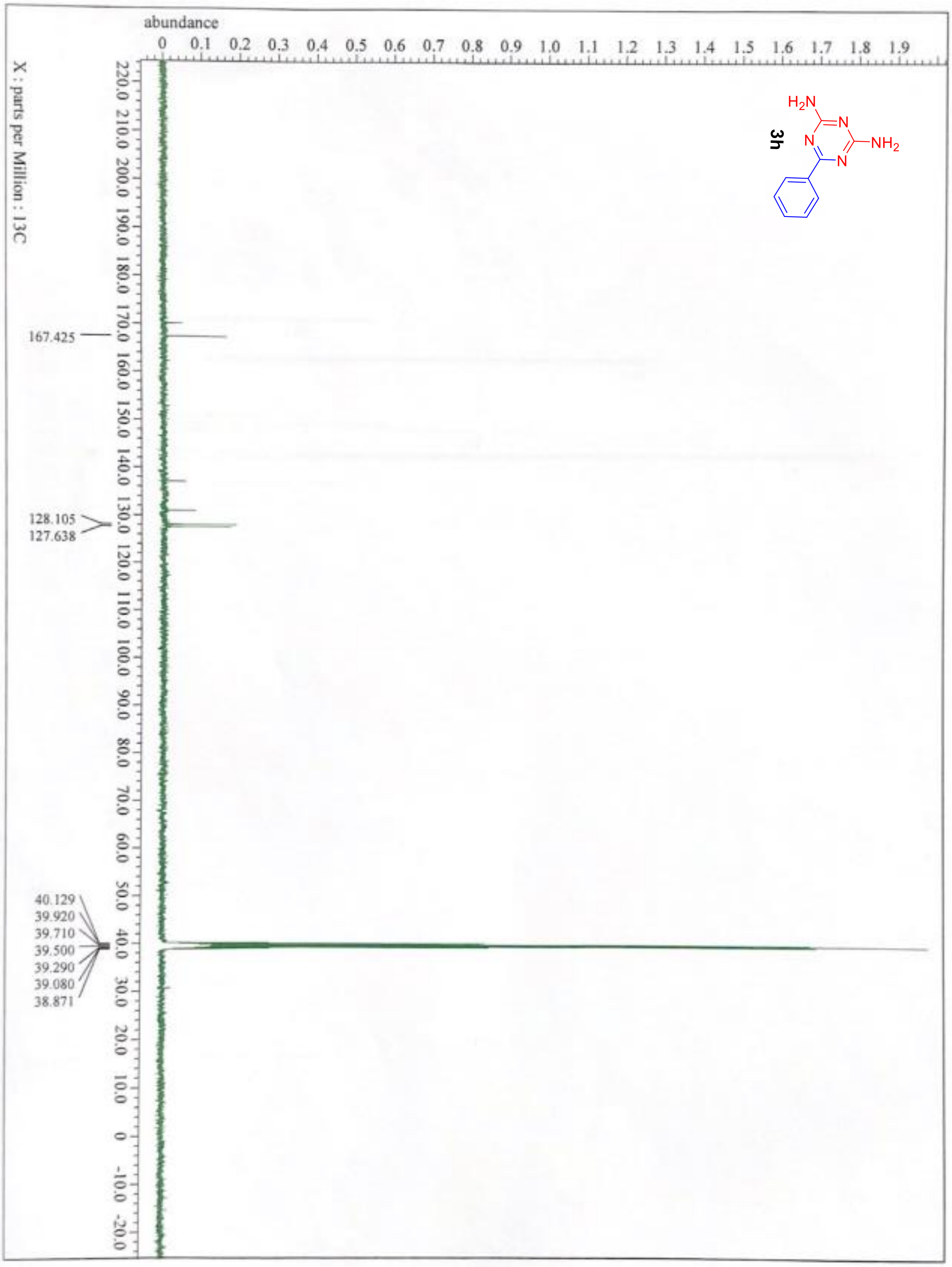
2.481
2.067
X : parts per Million : 1H



abundance
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X : parts per Million : 13C
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
167.425
128.105
127.638
40.129
39.920
39.710
39.500
39.290
39.080
38.871
3h
H2N
NH2
N